Property values tagged with IC are from the ZIC/VINITI data file
provided by InfoChem.

STRUCTURE FILE UPDATES: 23 JUN 2004 HIGHEST RN 698346-19-9
DICTIONARY FILE UPDATES: 23 JUN 2004 HIGHEST RN 698346-19-9

TSCA INFORMATION NOW CURRENT THROUGH JANUARY 6, 2004

Please note that search-term pricing does apply when
conducting SmartSELECT searches.

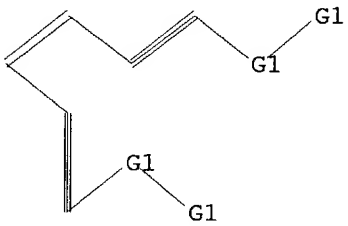
Crossover limits have been increased. See HELP CROSSOVER for details.

Experimental and calculated property data are now available. For more
information enter HELP PROP at an arrow prompt in the file or refer
to the file summary sheet on the web at:
http://www.cas.org/ONLINE/DBSS/registryss.html

=>
Uploading C:\Program Files\Stnexp\Queries\913924.str

L1 STRUCTURE UPLOADED

=> d l1
L1 HAS NO ANSWERS
L1 STR




M

G1 O,S,N,CH2,Cy

Structure attributes must be viewed using STN Express query preparation.

=> s l1
SAMPLE SEARCH INITIATED 14:28:56 FILE 'REGISTRY'
SAMPLE SCREEN SEARCH COMPLETED - 287 TO ITERATE

100.0% PROCESSED 287 ITERATIONS 0 ANSWERS
SEARCH TIME: 00.00.01

FULL FILE PROJECTIONS: ONLINE **COMPLETE**
BATCH **COMPLETE**
PROJECTED ITERATIONS: 4724 TO 6756
PROJECTED ANSWERS: 0 TO 0

L2 0 SEA SSS SAM L1

=> s l1 sss full
FULL SEARCH INITIATED 14:29:02 FILE 'REGISTRY'
FULL SCREEN SEARCH COMPLETED - 5762 TO ITERATE

100.0% PROCESSED 5762 ITERATIONS 3 ANSWERS
SEARCH TIME: 00.00.01

L3 3 SEA SSS FUL L1

=> file caplus
COST IN U.S. DOLLARS SINCE FILE ENTRY TOTAL SESSION
FULL ESTIMATED COST 155.42 155.63

FILE 'CAPLUS' ENTERED AT 14:29:08 ON 25 JUN 2004
USE IS SUBJECT TO THE TERMS OF YOUR STN CUSTOMER AGREEMENT.
PLEASE SEE "HELP USAGETERMS" FOR DETAILS.


FILE COVERS 1907 - 25 Jun 2004 VOL 141 ISS 1
FILE LAST UPDATED: 24 Jun 2004 (20040624/ED)

This file contains CAS Registry Numbers for easy and accurate substance identification.

=> s l3
L4 1 L3

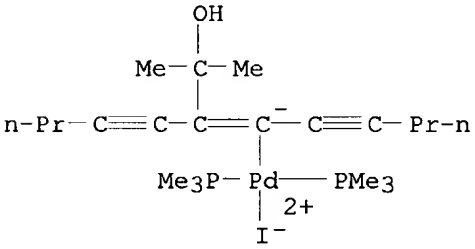
=> d l4 ibib abs hitstr

L4 ANSWER 1 OF 1 CAPLUS COPYRIGHT 2004 ACS on STN
ACCESSION NUMBER: 1995:486657 CAPLUS
DOCUMENT NUMBER: 122:314826
TITLE: Steric control of oxidative trimerization of alkynyl ligands in trimethylphosphine palladium complexes
AUTHOR(S): Klein, Hans-Friedrich; Zettel, Bernd D.
CORPORATE SOURCE: Eduard-zintl-Inst. Anorganische Chem., Technischen Hochschule Darmstadt, Darmstadt, D-64287, Germany
SOURCE: Chemische Berichte (1995), 128(4), 343-50
CODEN: CHBEAM; ISSN: 0009-2940
PUBLISHER: VCH
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 122:314826
AB Alkynylpalladium compds. trans-PdX(C.tplbond.CR)(PMe3)2 [R = CMe3, X = Cl (1), I (19); R = CMe2OH, X = Cl (2), Br (10), I (11); R = c-Hex, X = Cl (3), Br (12), I (13); R = CHMe2, X = Br (4); R = CH2SiMe3, X = Cl (5), Br (14), I (15); R = COOEt, X = Br (6), I (7); R = Ph, X = Cl (8), I (17); R = Pr, X = N3 (16), I (20); R = n-Hex, X = I (21); R = SiPh3, X = Br (22)] and trans-PdX(C.tplbond.CR)(PBu3)2 [R = SiMe3, X = Cl (9), I (18)] as well as trans-PdX(C.tplbond.CR)(PPh3)2 [R = CMe3, X = Br (23); R = CH2SiMe3, X

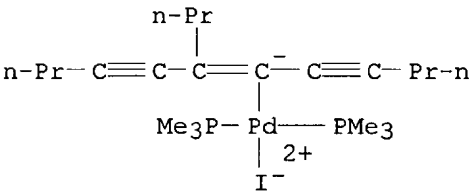
= Br (24), I (25)] were prepared by known methods. Thermal decomposition between
120 and 160° results in a selective transformation only with trimethylphosphine complexes 1, 2, 10-13, and 19. Oxidative trimerization of the alkynyl groups C.tplbond.CCMe2R' and C.tplbond.C(c-Hex) affording the enediynyl compds. trans-PdX[C(C.tplbond.CCMe2R'):C(C.tplbond.CMe2R')CMe2R'](PMe3)2 [R' = Me, X = Cl (26), I (27); R' = OH, X = Cl (28), Br (29), I (30)] and trans-PdX{C[C.tplbond.C(c-Hex)]:C[C.tplbond.C(c-Hex)](c-Hex)}(PMe3)2 [X = Br (31), I (32)] appears to be controlled by balanced steric demands of P and alkynyl substituents. The steric control was studied by melting transformable monoalkynyl complex trans-PdI(C.tplbond.CCMe2OH)(PMe3)2 (11) with nontransformable complex trans-PdI[C.tplbond.C(nPr)](PMe3)2 (20) to give a mixture (A) of transformed complexes with mixed substituents R. Similar results were obtained in other mixts., when transformable PdBr(C.tplbond.CSiMe3)(PMe3)2[1] is heated with the nontransformable complexes PdBr[C.tplbond.C(nPr)](PMe3)2[1] and 20 (mixture B) or transformable PdBr[C.tplbond.C(c-Hex)](PMe3)2 (12) with nontransformable PdBr[C.tplbond.C(nPr)](PMe3)2[1] (mixture C).

IT **163494-82-4P 163494-83-5P 163494-85-7P**
RL: PRP (Properties); SPN (Synthetic preparation); PREP (Preparation)
(Steric control of thermal oxidative trimerization of alkynyl ligands in trimethylphosphine palladium complexes with characterization by IR and NMR spectroscopy)

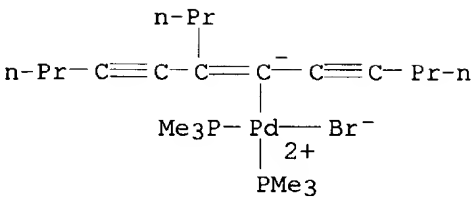
RN 163494-82-4 CAPLUS
CN Palladium, [2-(1-hydroxy-1-methylethyl)-1-(1-pentynyl)-1-hepten-3-ynyl]iodobis(trimethylphosphine)-, [SP-4-3-(E)]- (9CI) (CA INDEX NAME)



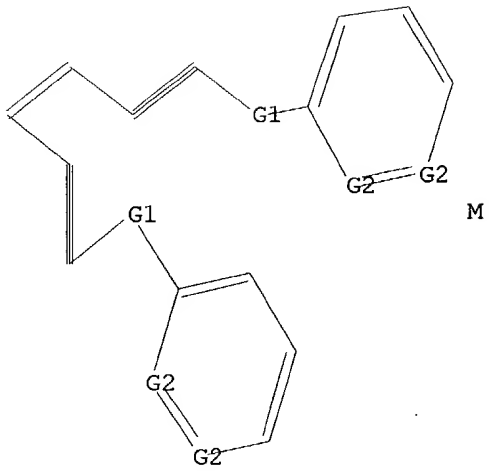
RN 163494-83-5 CAPLUS
CN Palladium, iodo[1-(1-pentynyl)-2-propyl-1-hepten-3-ynyl]bis(trimethylphosphine)-, [SP-4-3-(Z)]- (9CI) (CA INDEX NAME)



RN 163494-85-7 CAPLUS
CN Palladium, bromo[1-(1-pentynyl)-2-propyl-1-hepten-3-ynyl]bis(trimethylphosphine)-, [SP-4-3-(Z)]- (9CI) (CA INDEX NAME)



R



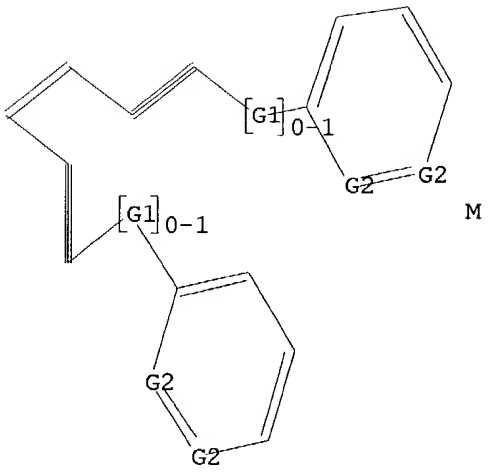

M

G1 O,S,N,CH2,Cy

G2 C,N

Structure attributes must be viewed using STN Express query preparation.

```
=> s l5 sss full
FULL SEARCH INITIATED 14:33:24 FILE 'REGISTRY'
FULL SCREEN SEARCH COMPLETED -  20622 TO ITERATE

100.0% PROCESSED   20622 ITERATIONS                                0 ANSWERS
SEARCH TIME: 00.00.01

L6             0 SEA SSS FUL L5

=>
Uploading C:\Program Files\Stnexp\Queries\913924.str

L7       STRUCTURE UPLOADED

=> d l7
L7 HAS NO ANSWERS
L7                STR
```




G1 O,S,N,CH2,Cy

G2 C,N

Structure attributes must be viewed using STN Express query preparation.

=> s l7 sss full
FULL SEARCH INITIATED 14:34:31 FILE 'REGISTRY'
FULL SCREEN SEARCH COMPLETED - 118701 TO ITERATE

100.0% PROCESSED 118701 ITERATIONS 13 ANSWERS
SEARCH TIME: 00.00.02

L8 13 SEA SSS FUL L7

=> file caplus

| COST IN U.S. DOLLARS | SINCE FILE ENTRY | TOTAL SESSION |
|---|---|---|
| FULL ESTIMATED COST | 312.94 | 474.64 |

| DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS) | SINCE FILE ENTRY | TOTAL SESSION |
|---|---|---|
| CA SUBSCRIBER PRICE | 0.00 | -0.69 |

FILE 'CAPLUS' ENTERED AT 14:34:38 ON 25 JUN 2004
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PLEASE SEE "HELP USAGETERMS" FOR DETAILS.


FILE COVERS 1907 - 25 Jun 2004 VOL 141 ISS 1

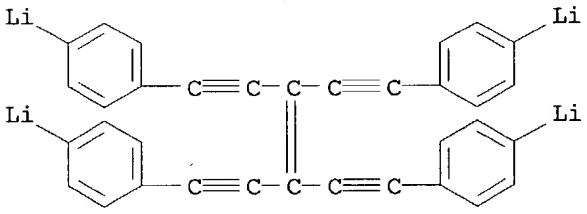
09/913,924

FILE LAST UPDATED: 24 Jun 2004 (20040624/ED)

This file contains CAS Registry Numbers for easy and accurate substance identification.

=> s l8
L9 2 L8

L9 ANSWER 1 OF 2 CAPLUS COPYRIGHT 2004 ACS on STN
ACCESSION NUMBER: 1999:365203 CAPLUS
DOCUMENT NUMBER: 131:191533
TITLE: Nonlinear optical properties of lithium-containing derivatives
AUTHOR(S): Papadopoulos, Manthos G.; Screttas, Ceorgios C.; Raptis, Stavros G.; Theologitis, Markos M.
CORPORATE SOURCE: Institute or Organic and Pharmaceutical Chemistry, National Helenic Research Foundation, Athens, Greece
SOURCE: Proceedings of SPIE-The International Society for Optical Engineering (1999), 3623(Organic Photonic Materials and Devices), 270-278
CODEN: PSISDG; ISSN: 0277-786X
PUBLISHER: SPIE-The International Society for Optical Engineering
DOCUMENT TYPE: Journal
LANGUAGE: English
AB The polarizability and 1st and 2nd hyperpolarizabilities of several 4,4'-disubstituted trans-stilbene (tSB) derivs., which include the NO2 group as an acceptor (A) and several Li containing donors (D) were computed. Ab initio theory using a 6-31G basis set at the SCF and MP2 levels was sued to optimize the structure of tSB and the disubstituted derivative which includes the NO2 (A) and the NLi2 (D). Their polarizabilities and hyperpolarizabilities also were computed at the SCF level. MP2 theory was used to assess the effect of correlation on the largest polarizability and 2nd hyperpolarizability components of the above compds. The preset results, together with the authors' recent work show that the 2nd hyperpolarizabilities of some lithiated derivs. depend quite a lot on the mol. geometries and lithiation leads to a big increase of the hyperpolarizabilities of the resulting derivs. Probably at lest some of the lithiated derivs. are very likely to be useful for nonlinear optical applications.
IT **222173-77-5**
RL: PRP (Properties)
(nonlinear optical properties of lithium-containing derivs.)
RN 222173-77-5 CAPLUS
CN Lithium, [μ-[[3,4-bis[(4-lithiophenyl)ethynyl]-3-hexene-1,5-diyne-1,6-diyl]di-4,1-phenylene]]di- (9CI) (CA INDEX NAME)




REFERENCE COUNT: 27 THERE ARE 27 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

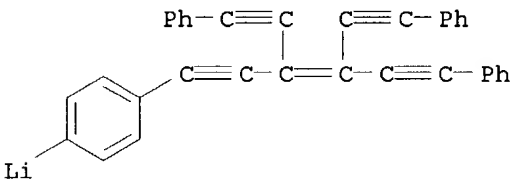
L9 ANSWER 2 OF 2 CAPLUS COPYRIGHT 2004 ACS on STN
ACCESSION NUMBER: 1999:123367 CAPLUS
DOCUMENT NUMBER: 130:267476
TITLE: The polarizability and the second hyperpolarizability of tetrakis(phenylethynyl)ethene and several of its lithiated derivatives
AUTHOR(S): Theologitis, M.; Screttas, G. C.; Raptis, S. G.; Papadopoulos, M. G.

CORPORATE SOURCE: Chemical Engineering Department, National Technical University of Athens, Athens, 15773, Greece
SOURCE: International Journal of Quantum Chemistry (1999), 72(3), 177-187
CODEN: IJQCB2; ISSN: 0020-7608
PUBLISHER: John Wiley & Sons, Inc.
DOCUMENT TYPE: Journal
LANGUAGE: English

AB The polarizability ($\alpha$) and the second hyperpolarizability ($\gamma$) of tetrakis(phenylethynyl)ethene (TPEE) are compared and analyzed in connection with the properties ($\alpha$, $\gamma$) of a series of selected/designed mols. having different conjugation patterns. Several lithiated derivs. of TPEE are designed and shown to have very enhanced second hyperpolarizabilities; for example, one of the lithiated TPEE has a 1.6 + 103 times larger second hyperpolarizability than that of benzene. The potential of the proposed derivs. for applications in photonics is noted. The polarizabilities and the hyperpolarizabilities of the considered mols. have been computed employing the PM3 method which has been proven to be adequate for the present comparative study.

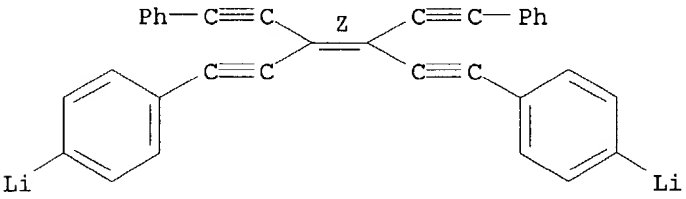
IT **222173-74-2 222173-75-3 222173-76-4 222173-77-5 222173-78-6 222173-79-7 222173-80-0 222173-81-1 222173-82-2 222173-83-3 222173-84-4 222173-85-5 222174-20-1**
RL: PRP (Properties)
(polarizability and second hyperpolarizability of)

RN 222173-74-2 CAPLUS
CN Lithium, [4-[6-phenyl-3,4-bis(phenylethynyl)-3-hexene-1,5-diynyl]phenyl]- (9CI) (CA INDEX NAME)

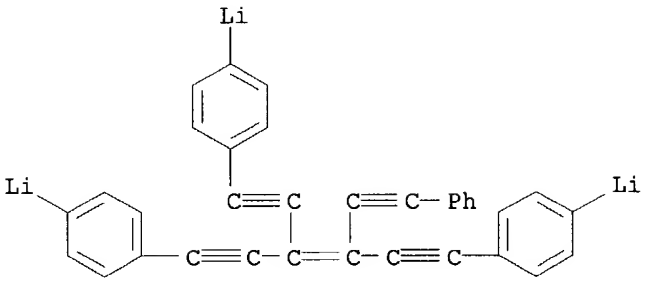


RN 222173-75-3 CAPLUS
CN Lithium, [μ-[[(3Z)-3,4-bis(phenylethynyl)-3-hexene-1,5-diyne-1,6-diyl]di-4,1-phenylene]]di- (9CI) (CA INDEX NAME)

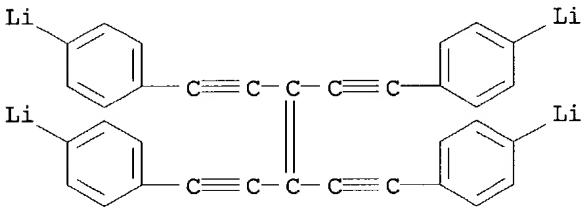
Double bond geometry as shown.



RN 222173-76-4 CAPLUS
CN Lithium, [μ-[[3-[(4-lithiophenyl)ethynyl]-4-(phenylethynyl)-3-hexene-1,5-diyne-1,6-diyl]di-4,1-phenylene]]di- (9CI) (CA INDEX NAME)

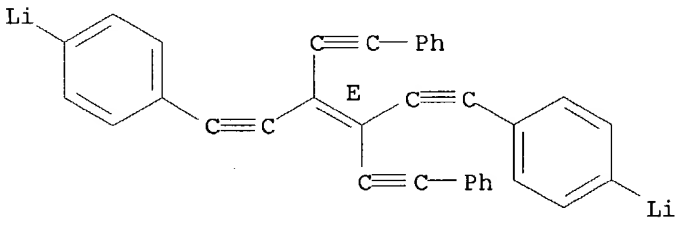


RN 222173-77-5 CAPLUS
CN Lithium, [μ-[[3,4-bis[(4-lithiophenyl)ethynyl]-3-hexene-1,5-diyne-1,6-diyl]di-4,1-phenylene]]di- (9CI) (CA INDEX NAME)

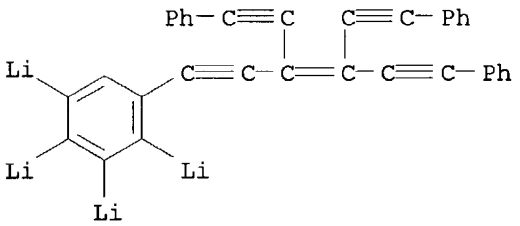


RN 222173-78-6 CAPLUS
CN Lithium, [μ-[[(3E)-3,4-bis(phenylethynyl)-3-hexene-1,5-diyne-1,6-diyl]di-4,1-phenylene]]di- (9CI) (CA INDEX NAME)

Double bond geometry as shown.

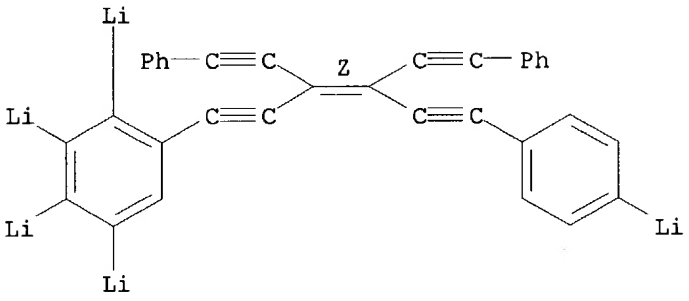


RN 222173-79-7 CAPLUS
CN Lithium, [μ4-[5-[6-phenyl-3,4-bis(phenylethynyl)-3-hexene-1,5-diynyl]-1,2,3,4-benzenetetrayl]]tetra- (9CI) (CA INDEX NAME)



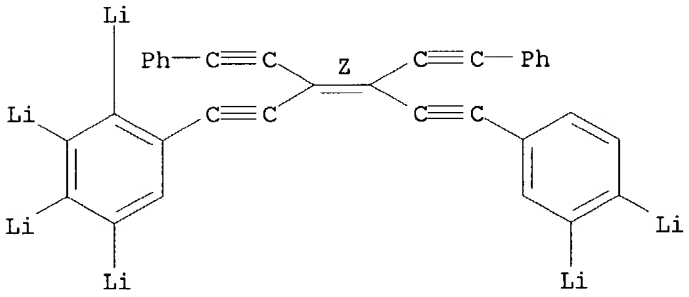
RN 222173-80-0 CAPLUS
CN Lithium, [μ4-[5-[(3Z)-6-(4-lithiophenyl)-3,4-bis(phenylethynyl)-3-hexene-1,5-diynyl]-1,2,3,4-benzenetetrayl]]tetra- (9CI) (CA INDEX NAME)

Double bond geometry as shown.



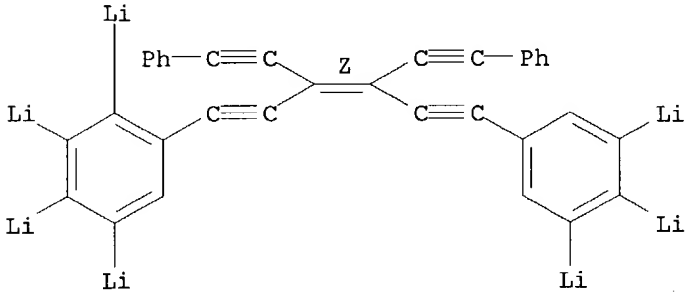
RN 222173-81-1 CAPLUS
CN Lithium, [μ4-[5-[(3Z)-6-(3,4-dilithiophenyl)-3,4-bis(phenylethynyl)-3-hexene-1,5-diynyl]-1,2,3,4-benzenetetrayl]]tetra- (9CI) (CA INDEX NAME)

Double bond geometry as shown.



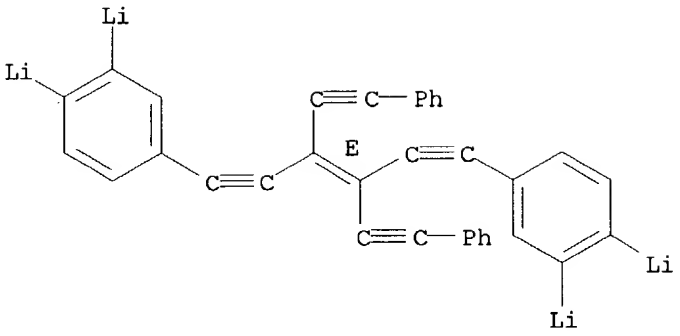
RN 222173-82-2 CAPLUS
CN Lithium, [μ4-[5-[(3Z)-3,4-bis(phenylethynyl)-6-(3,4,5-trilithiophenyl)-3-hexene-1,5-diynyl]-1,2,3,4-benzenetetrayl]]tetra- (9CI) (CA INDEX NAME)

Double bond geometry as shown.



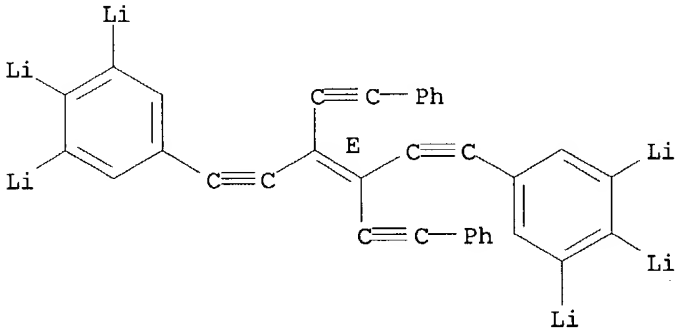
RN 222173-83-3 CAPLUS
CN Lithium, [μ4-[[(3E)-3,4-bis(phenylethynyl)-3-hexene-1,5-diyne-1,6-diyl]di-4,1,2-benzenetriyl]]tetra- (9CI) (CA INDEX NAME)

Double bond geometry as shown.



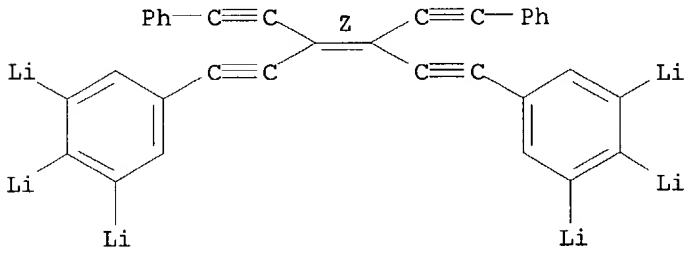
RN 222173-84-4 CAPLUS
CN Lithium, [μ6-[[(3E)-3,4-bis(phenylethynyl)-3-hexene-1,5-diyne-1,6-diyl]di-5,1,2,3-benzenetetrayl]]hexa- (9CI) (CA INDEX NAME)

Double bond geometry as shown.



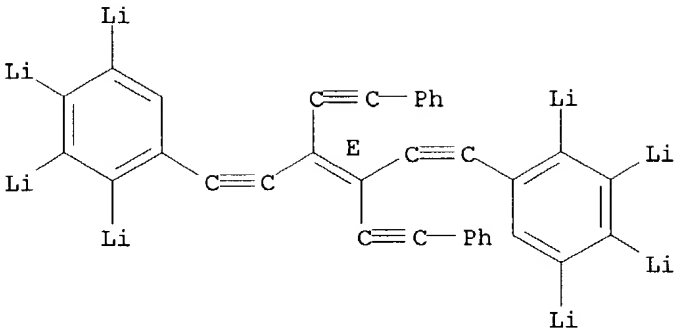
RN 222173-85-5 CAPLUS
CN Lithium, [μ6-[[(3Z)-3,4-bis(phenylethynyl)-3-hexene-1,5-diyne-1,6-diyl]di-5,1,2,3-benzenetetrayl]]hexa- (9CI) (CA INDEX NAME)

Double bond geometry as shown.



RN 222174-20-1 CAPLUS
CN Lithium, [μ8-[[(3E)-3,4-bis(phenylethynyl)-3-hexene-1,5-diyne-1,6-diyl]di-5,1,2,3,4-benzenepentayl]]octa- (9CI) (CA INDEX NAME)

Double bond geometry as shown.




REFERENCE COUNT: 40 THERE ARE 40 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

=>